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Evaluation of the Prompt Fission Neutron Spectrum of Thermal-neutron Induced Fission in U-235

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Abstract

A new evaluation of the prompt fission neutron spectra (PFNS) for the neutron-induced fission of the U-235 nucleus is presented. By using differential data as "shape data" good consistency was achieved between selected sets of differential data. A fit of differential PFNS data with the generalised least-squares method using the GANDR code allowed the estimation of the uncertainties and correlations. All experimental data were consistently fitted in a model independent way giving a PFNS average energy of 2.000 MeV with an estimated 9 keV uncertainty.

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Keywords: PFNS, neutron induced, fission

1. INTRODUCTION

The energy spectrum of prompt neutrons emitted in fission plays an important role in many applications in nuclear science and technology including reactor applications, criticality and benchmarking calculations. The conclusion from the Consultants Meeting on "Prompt Fission Neutron Spectra of Major Actinides", which was held at the IAEA Headquarters in Vienna, Austria, in November 2008 and summarized in a report by Capote *et al.* (2009), was that the prompt fission neutron spectra (PFNS) in the present evaluated nuclear data libraries are inadequate and that their uncertainty estimates are unrealistic. As a consequence, a Coordinated Research Project (CRP) on Prompt Fission Neutron Spectra for Actinides was initiated by the IAEA in 2010. At the same time, significant efforts have been made by the Neutron Standards Evaluation Group to undertake a new evaluation of the PFNS in the thermal-neutron-induced fission of the ^{235}U nucleus that could be proposed as a secondary reference neutron spectrum. The on-going work is summarized in meeting reports by Pronyaev *et al.* (2011), Pronyaev *et al.* (2013). Reasons for the small uncertainties reported by several evaluators as a result of direct fitting of the measured PFNS data have been studied recently by Neudecker *et al.* (2013). The PFNS and associated covariances for incident neutron energies up to 30 MeV

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are being also investigated as part of the CIELO project, described by Chadwick *et al.* (2014), with the aim of creating an international database of evaluated nuclear reaction data files. In the present work we focus on the evaluation of the PFNS of thermal-neutron-induced fission of the ^{235}U nucleus. The evaluation is carried out by a non-model fit of measured differential data using the Generalised Least-Squares method (GLSQ) in the GANDR code, developed by Muir (2001).

2. EXPERIMENTAL DATA

2.1. Measured Differential Data

As a starting point the selected experimental data with uncertainty analysis were adopted as prepared by Pronyaev for the CRP on PFNS. Further details on the data and the selection process can be found on the CRP PFNS (2011) web page. A comprehensive discussion on differential data selection from the EXFOR database is available on the CIELO-IAEA (2014) web page. The differential data sets (listed in backward chronological order) that are recommended for fitting the shape of the thermal-neutron induced PFNS of ^{235}U are listed in Table 1.

Table 1. List of measured differential PFNS data sets.

Author	EXFOR No.	Scaling factor	Type of data	Comments
Vorobyev *et al.* (2014)	41597002	1.5250	ratio, absolute	
Kornilov *et al.* (2011)	31692006	1.5720	ratio, absolute	
Wang Yufeng *et al.* (1989)	32587002	6.4433	spectrum, shape	discarded below 1.3 MeV
Lajtai *et al.* (1985)	30704003	1.0125	spectrum, absolute	discarded above 0.2 MeV
Starostov *et al.* (1983)	40872007	1.6436	ratio, absolute	
Nefedov *et al.* (1983)	40871011	1.6128	ratio, absolute	
Nefedov *et al.* (1983)	40871012	1.6571	ratio, absolute	
Boytsov *et al.* (1983)	40873004	1.0039	spectrum, absolute	discarded above 2.7 MeV

Four data points above 2.7 MeV in the data by Boytsov *et al.* (1983) were discarded, as they were discarded also in a subsequent publication by the same authors (see Starostov *et al.* (1985)). The rest of the data of Boytsov *et al.* (1983) were taken because they were provided to EXFOR by the author in numerical form, while the Starostov *et al.* (1985)) data in EXFOR were digitised from a graph in a publication. The data were measured as ratios to ^{252}Cf but converted to ratio with a Maxwellian spectrum with temperature 1.313 MeV, assuming the ^{252}Cf spectrum was also a Maxwellian with temperature 1.42 MeV. A correction for the standard ^{252}Cf spectrum was made. The data by Lajtai *et al.* (1985) above 0.2 MeV were deemed unreliable because of very large corrections (more than ~50% at some energies) that had to be applied due to the use of a thick Li-glass detector in the measurements. The data by Wang Yufeng *et al.* (1989) below 1.3 MeV were excluded due to the unphysical shape of the measured spectrum, which seems to be caused by the employed detector efficiency (the efficiency at those energies was extrapolated, not measured). Also, uncertainties of the last two points in the latter data set were doubled and tripled, respectively, for statistical consistency with other data; the uncertainties in the last two points in the data by Kornilov *et al.* (2011) were doubled for the same reason. Even after these uncertainty modifications we can see from Fig. 1 that experimental differential data above 10 MeV are discrepant, therefore those data were discarded in the least-squares analysis.

3. FITTING OF THE FISSION SPECTRA

3.1. Using measured differential data as shape data

The majority of the measured ^{235}U PFNS differential data are absolute ratios to the ^{252}Cf spontaneous fission spectrum as can be seen from Table 1. Ratio measurements allow reduction of the uncertainty of measured PFNS, however, what is really measured is the ratio of the energy-dependent neutron yield $Y(E) = \overline{\nu}\chi(E)$, where χ is a normalised PFNS (by definition); i.e. the shape of the PFNS. The absolute normalization of such data obviously depends on the assumed (not measured) ratio of multiplicities $\overline{\nu}(^{235}U)/\overline{\nu}(^{252}Cf)$. The measured multiplicity ratio

should be calculated by integration over all outgoing neutron energies, and therefore strongly depends on the outgoing neutron energies of measurements. However, $\overline{\nu}$ can be measured much more accurately by different experiments, therefore we need to evaluate the "shape" information only (i.e. $\chi(E)$ in the yield). For that reason we can treat all differential data as "shape" data with floating normalization. In practice this means that we can scale each data set arbitrarily to a common reference so as to maximize the consistency between them as discussed by Smith *et al.* (2015) . In this work such common reference for scaling is taken to be the basis function described in Section 3.2. The ENDF-6 format requirement of normalisation on the PFNS (and its covariance matrix) is applied *a-posteriori*, making some assumptions about the high- and low-energy tails of the spectrum where no differential data exist.

3.2. Basis function for scaling and extrapolation

The data in EXFOR are given in different representations. To bring all data to the same basis, each data set was converted to "shape" spectrum ratio to a Maxwellian spectrum with temperature 1.32 MeV, scaled to match a chosen basis function by minimising the squares of the relative differences between the measured values and the basis function. The basis function $f(E)$ was defined as a linear combination of a Maxwellian function f_M and a Watt function f_W, which was found to represent the data reasonably well.

$$f(E) = w_M f_M(E, E_M) + (1 - w_M) f_W(E, a_W, b_W)$$
$$f_M(E, E_M) = K_M \sqrt{E} e^{-E/E_M}$$

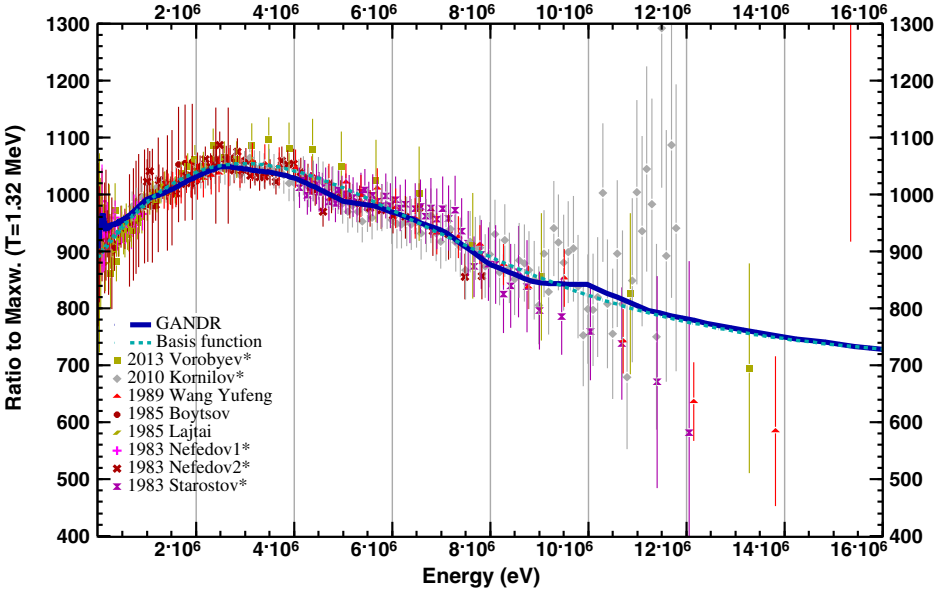

Fig. 1. Fitted spectra in linear energy scale (bold blue line) and "prior" basis function (dashed cyan line) in comparison with rescaled "shape" differential data (symbols) displayed as ratios to a Maxwellian with temperature 1.32 MeV .

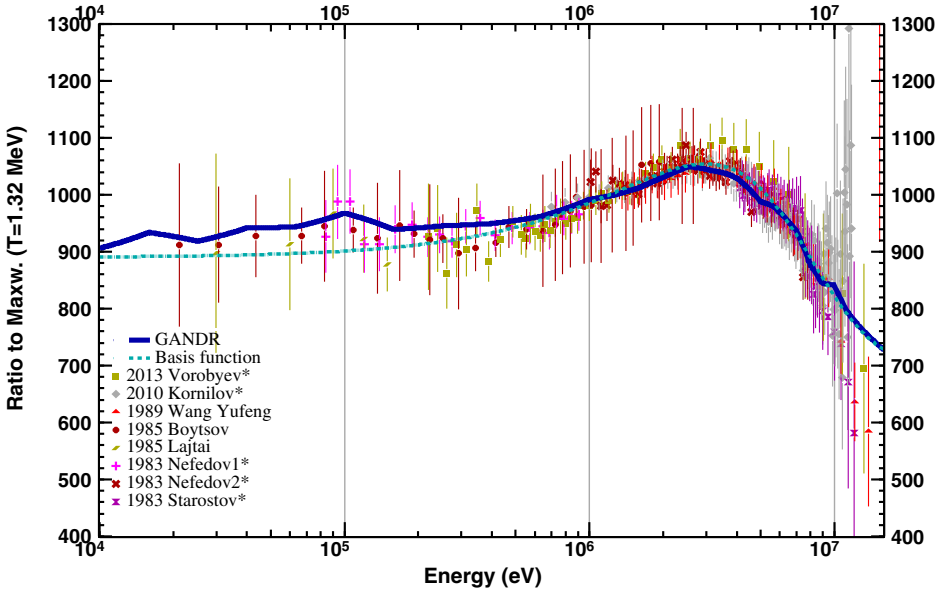

Fig. 2. Fitted spectra in logarithmic energy scale (bold blue line) and "prior" basis function (dashed cyan line) in comparison with rescaled "shape" differential data (symbols) displayed as ratios to a Maxwellian with temperature 1.32 MeV (symbols).

$$f_W(E, a_W, b_W) = K_W e^{-E/a_W} \sinh \sqrt{b_W E} \tag{1}$$

where w_M is the weight of the Maxwellian contribution, $E_M = kT$ is the temperature of the Maxwellian, a_W, b_W are the parameters of the Watt function and K_M, K_W are normalisation constants, which can be expressed analytically.

The fitted basis function (1) is only used for scaling the experimental data and for extrapolation of differential data beyond the range where experimental data are available and statistically consistent (i.e. above 20 keV and below ~10 MeV. Therefore, the basis function serves only as an auxiliary mathematical tool. The fitted parameters of the basis function derived by Trkov *et al.* (2015) are: $w_M = 0.7424$, $E_M = 1.316$ MeV, $a_W = 0.6859$ MeV, and $b_W = 9.366$ MeV^{-1}. These parameters are not unique, but the function serves the purpose it was designed for, as discussed above. The fitting of the basis function parameters made use of the information derived from reactor dosimetry cross-section data (i.e. average cross-section ratio in ^{252}Cf(sf) and ^{235}U(n$_{th}$,f) fission spectra) for high-threshold dosimetry reactions with effective energy threshold above 8 MeV. This information was used to fix the PFNS shape at higher neutron outgoing energies, where very poor differential data exist. The impact of this modification (through the normalization) at lower neutron outgoing energies was found by Trkov *et al.* (2015) to be negligible.

After re-scaling the combined experimental data sets cover more than 99 % of the contribution to the integral. Since the scaling is done to an arbitrary reference basis function, the spectrum integral after the fitting procedure is not necessarily equal to one, even if the chosen basis function is normalised, as in our case. This additional scaling factor was 1.0125.

The scaling factors for each data set are listed in the Table 1. These are values with which the EXFOR entries have to be divided to match the final fitted curve. For the ratio measurements the factors include the $\overline{\nu}(^{252}\mathrm{Cf})/\overline{\nu}(^{235}\mathrm{U})$ ratio

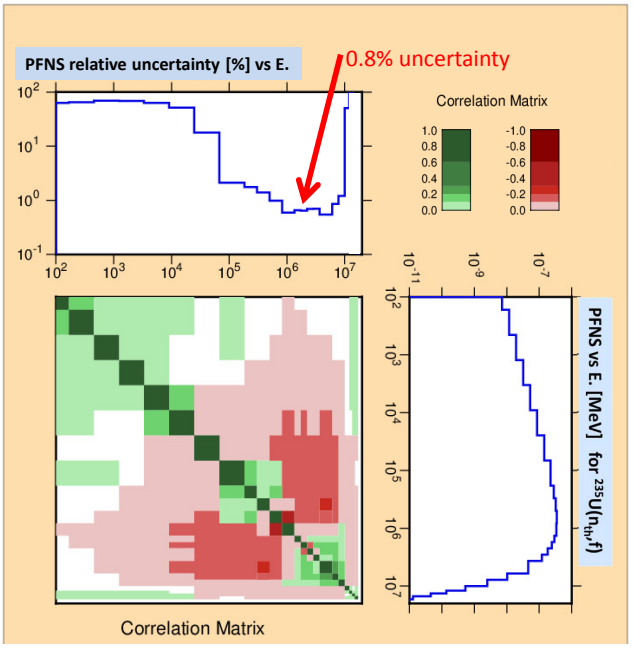

Fig. 3. Uncertainty and correlation matrix of the normalized GANDR fitted PFNS.

value. Note that the precise value of this ratio is not needed; differences in the scaling factors from this value reflect the differences in the geometry of the measurement set-up of the ^{252}Cf and ^{235}U spectra, the corresponding detector efficiencies and any other unaccounted corrections.

3.3. Generalised Least Squares Fit

The fitting was performed with the GANDR system of Muir (2001), which uses the generalised least-squares technique. It calculates the parameters of a piecewise-linear correction function defined on a fixed energy grid, applied on an input prior. The prior was "non-informative", having the shape of the previously defined basis function but an assigned uncorrelated uncertainty of 100%. This means that the prior had practically no influence on the final solution in the energy region where measured data were available. The advantage of GANDR is that the fitted function is defined at every point and does not require pre-processing and transformation of experimental data to a fixed energy grid. In comparison, it produces a smoother function on output, but cannot follow short-range structures in the data.

The ratios of the evaluated spectra to the pure Maxwellian at temperature 1.32 MeV are compared in Figs. 1 and 2 in linear and logarithmic energy scale, respectively. The basis function is also depicted. Below 20 keV and above 10 MeV the evaluation agrees with the basis function that was taken as prior, as expected.

Normalisation of the spectrum is trivial: by definition the integral must be equal to one. Normalisation of the covariance matrix is less straightforward. The covariance matrix is evaluated in terms of absolute uncertainties over specified energy intervals. In a normalised covariance matrix the sum of elements of any row or column equals zero. Since a residual normalisation uncertainty is present in the covariance matrix obtained directly from the fitting procedure, the zero-sum property is not respected. The procedure for covariance matrix normalisation was applied as given by Equation (35.2) in the ENDF Manual (2012).

The uncertainty estimate in the unnormalised spectrum over a broad energy range around the peak of the spectrum is about 3.5 %. The evaluated shape uncertainty after normalisation and the corresponding correlation matrix are shown in Fig. 3. The minimum uncertainty near the peak of the normalised PFNS is about 0.8 %, due to the approximate uncertainty analysis used in the input. Further uncertainty analysis is required for a final evaluation. The uncertainty of the evaluated normalised PFNS goes back to the uncertainty of the prior in the region where no experimental data was considered. The derived average energy (with uncertainty of the last digit) is 2.000(9) MeV.

4. CONCLUSIONS

The fitting of the thermal-neutron-induced fission spectrum of ^{235}U using differential data was investigated using the GLSQ package GANDR. Using the differential data as "shape data", very good statistical consistency between different differential data sets is observed for outgoing neutron energies below 10 MeV. Available differential data define the evaluated spectra from 20 keV up to 10 MeV of outgoing neutron energy covering about 99% of the neutron emission probability. The mean neutron energy derived from the fitted PFNS is 2.000(9) MeV and is lower than the current ENDF/B-VII.1 value of 2.03 MeV.

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